



## **ACE001: Heavy-Duty Diesel Combustion**

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FY 2020 DOE Vehicle Technologies Office Annual Merit Review  
Advanced Combustion Engines (ACE)  
10:00 – 10:30 AM, Thursday, June 4, 2020

**Sponsor:** **U.S. Dept. of Energy, Office of Vehicle Technologies**

**Program Managers:** **Michael Weismiller, Gurpreet Singh**

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**ACE001**



# ACE001 Overview: Heavy-Duty Diesel Combustion

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## Timeline

3-year program in FY19-21 lab call

- Start date: FY19 Q1
- End date: FY21Q4
- Progress: 50% complete

## Budget

- Project funded by DOE/VTO:  
FY19 SNL+WERC: \$765k+\$115k  
FY20 SNL+WERC: \$650k+\$115k

## Barriers

From 21<sup>st</sup> Cent. Truck Partnership Roadmap & Tech. White Papers:

- Inadequate understanding of combustion & simulation from conventional diesel to LTC
- LTC aftertreatment integration
- Impact of future fuels on LTC

## Partners

- Wisconsin Engine Research Consultants, Lund University, Japan MPAT, ECN, TU Darmstadt, U of Connecticut, IFPE, Energies Nouvelles, Tech. U Eindhoven, U Erlangen
- 16 AEC MOU industry partners
- Project lead: Sandia (Musculus)

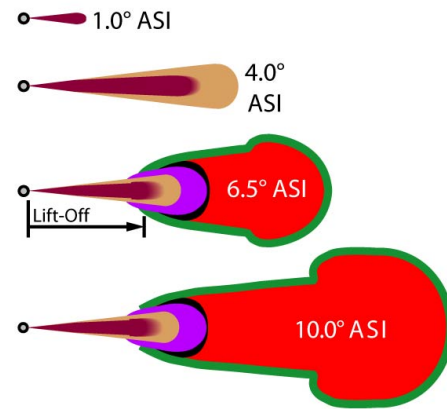


# ACE001 Relevance/Objectives: Heavy-Duty In-Cylinder Combustion

## Long-Term Objective

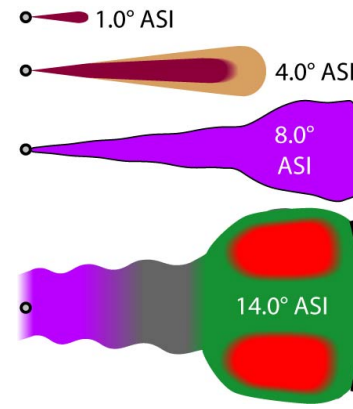
Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines

1997: **Conventional Diesel**  
(Single Injection)



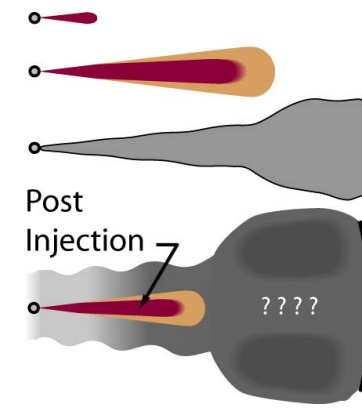
■ Liquid Fuel  
■ Pre-ignition Vapor Fuel  
■ First-Stage Ignition ( $\text{H}_2\text{CO}$ ,  $\text{H}_2\text{O}_2$ , CO, UHC)

2012: **LTC Diesel**  
(Single Injection)



■ Intermediate Ignition (CO, UHC)  
■ Second-Stage Ignition of Intermediate Stoichiometry or Diffusion Flame (OH)

2013+: **Multiple Injection**  
(Conventional & LTC)



■ Second-Stage Ignition of fuel-rich mixtures  
■ Soot or Soot Precursors (PAH)



# ACE001 Milestones: Heavy-Duty In-Cylinder Combustion

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## Long-Term Objective

**Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines**

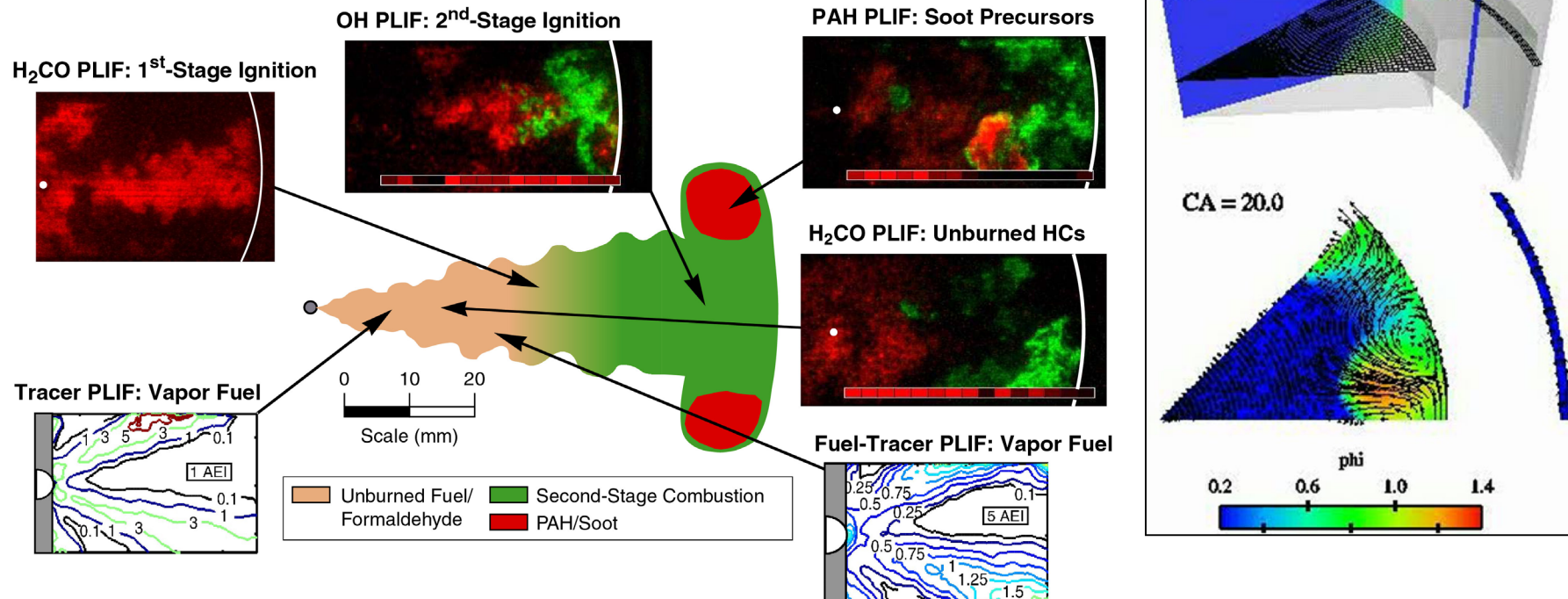
### Current Milestones/Objectives:

- ① SNL(Pickett) – Apply laser/imaging diagnostics to the transition from ignition to combustion for multiple injections
- ② SNL (Chen) – Use DNS simulation predictions to complement multiple injection experiments
- ③ WERC & SNL (Musculus/Hessel) – Use RANS simulation predictions to guide and complement multiple injection experiments
- ④ SNL (Musculus) – Develop diagnostics for multiple injection mixing and jet interactions



# ACE001 Approach: Optical imaging & CFD modeling of in-cylinder chemical/physical processes

- Combine planar laser-imaging diagnostics in an optical heavy-duty engine with multi-dimensional computer modeling (KIVA) to understand LTC combustion
- Transfer fundamental understanding to industry through working group meetings, individual correspondence, and publications





# ACE001: Collaboration & Coordination with Other Institutions

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- All work has been conducted under the Advanced Engine Combustion Working Group in cooperation with industrial partners
  - Cummins, Caterpillar, DDC, Mack Trucks, John Deere, GE, Paccar, International, Ford, GM, Daimler-Chrysler, ExxonMobil, ConocoPhillips, Shell, Chevron, BP, SNL, LANL, LLNL, ANL, ORNL, U. Wisconsin
- New research findings are presented at biannual meetings
- Tasks and work priorities are established in close cooperation with industrial partners
  - Both general directions and specific issues
- Industrial/University collaborations support experimental and simulation activities
  - Lund University in Sweden on laser-induced phosphorescence fuel tracing
  - Japan Institute of Maritime, Port, & Aviation Technology on diesel & dual-fuel natural gas
  - TU Darmstadt in Germany and U of Connecticut on DNS development and analysis
  - IFPEnergies Nouvelles in France, Tech. U Eindhoven in The Netherlands, and U Erlangen in Germany on high-speed laser-induced fluorescence imaging



# Responses to Reviewers' Comments from Previous Year

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Comment: *"It may be desirable and productive to add some more fundamental experiments to this research program to help isolate specific physical effects and reduce uncertainty where multiple physical phenomena come into play to affect the overall engine behavior ... spray diagnostics come to mind for fundamental experiments"*

Response: This year we included high-speed laser-induced fluorescence results for a combusting spray in a more fundamental constant-volume chamber facility, which provides a more controlled experiment with less uncertainty due to multiple phenomena occurs simultaneously.

Comment: *"it would be interesting to see similar progress on understanding the barriers to high-load LTC operation and, even more importantly, exploring pathways to overcome barriers ... limitations of the current optical engine hardware to high-pressure operation ... seems to indicate the need for bringing in additional or perhaps even new facilities"*

Response: The constant volume chamber facility of the laser-induced fluorescence experiments mentioned above also has capabilities for higher pressure than can be achieved in the engine.

Comment: *"Request more details on [collaborations], what results have been achieved from these collaborations, and what the future plans are for collaboration."*

Response: We have provided more details and references to collaborative efforts within the technical section of the presentation report.

Comment: *"It might be worthwhile to look at bringing on additional expertise to the project team (e.g., from researchers who have focused on heat transfer in academia or other places with appropriate diagnostics and analysis techniques to make more progress here)."*

Response: The heat transfer work is on pause for now, but we do plan to return to it in the future after addressing multiple injection issues described in the future plans of this report. When we do return to heat transfer, we will look for collaborators with complementary expertise.

Comment: *"This continues to be an exceptional program that combines state-of-the-art optical diagnostics in a diesel engine environment with multi-dimensional engine simulations to understand the combustion behavior in both conventional and low-temperature combustion (LTC) modes."*

Response: We will continue to follow this approach.



# ACE001: Technical Accomplishments and Progress

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- Accomplishments are described in the following 15 slides

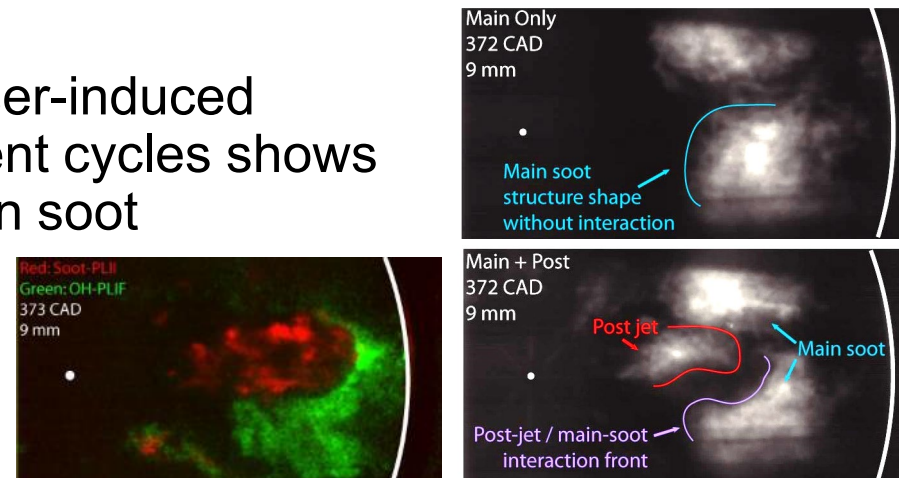
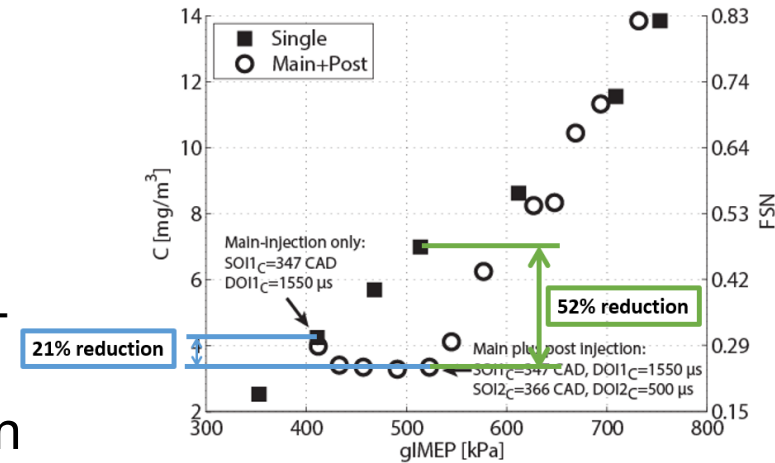
## Current Milestones/Objectives:

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- ② SNL (Chen) – Use DNS predictions to complement data from multiple injection experiments
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# ① Previous work on multiple injections points to importance of second injection disrupting first-injection residual jet

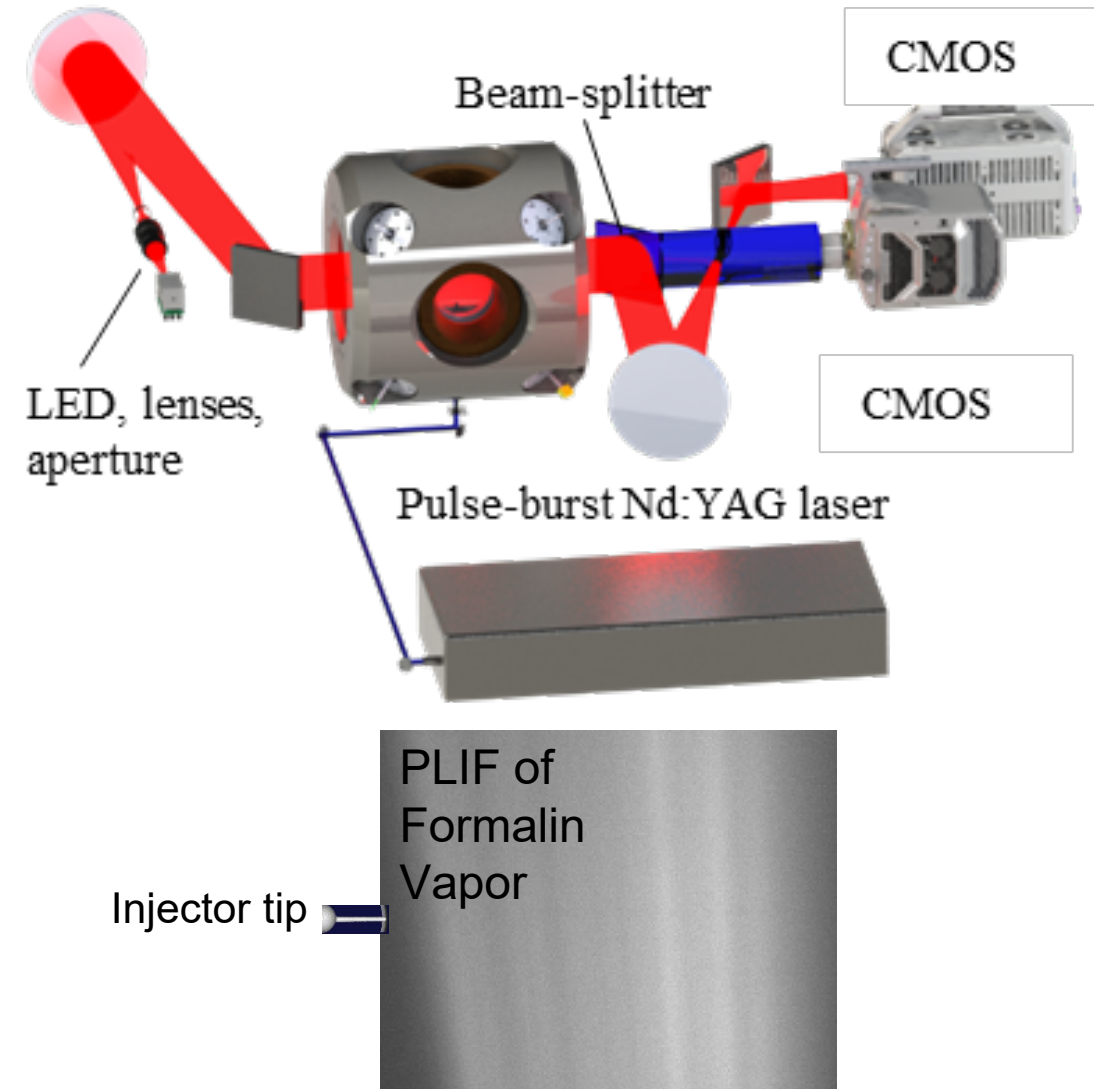
- Multiple injections can reduce both emissions and fuel consumption (FY13-18)
  - Reduce aftertreatment burden / allow more fuel-efficient condition
  - Directly reduce BSFC (SAE 2005-01-0928, 2001-01-0526, 2002-01-0502)
- Second injection interacts with end-of-injection residual of main-injection jet (FY14)
  - Ensemble-averaged soot planar laser-induced incandescence imaging from different cycles shows consistent disruption of first-injection soot
  - Single-cycle **OH fluorescence** provides evidence for **soot** oxidation by second injection in some cycles



**High-speed data from a single cycle would provide better cause-effect evidence of interactions between multiple injections**

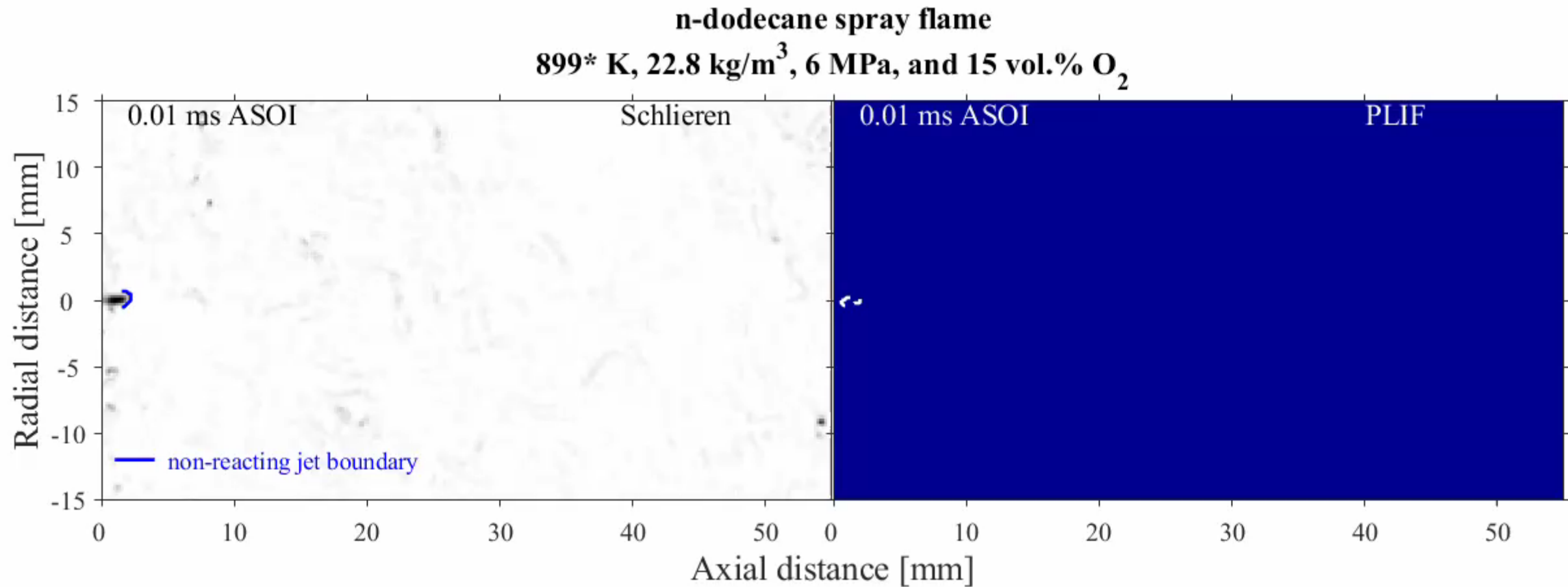
# ① 50 kHz planar 355-nm PLIF for multiple-injection ignition and soot precursor formation in a single cycle

- Pulse burst-mode 355-nm Nd:YAG laser
  - Spectral Energies Quasimodo
  - 300 sequential 70-mJ laser pulses @ 50 kHz
  - 55 mm x 0.5 mm laser sheet
- PLIF image using high-speed CMOS camera<sup>1</sup>
  - Non-intensified camera operates at 100,000 fps (twice the laser's repetition rate)
  - Dynamic background subtraction using “laser off” frame
- Schlieren (simultaneous) at 100 kHz
  - Pulsed infrared (centered at 850 nm) LED
  - Sensitive to temperature gradients along line-of-sight
- Laser energy distribution correction using formalin vapor
  - Energy distribution moves for each shot
  - Shot by shot correction
  - Photodiode records intensity of each shot



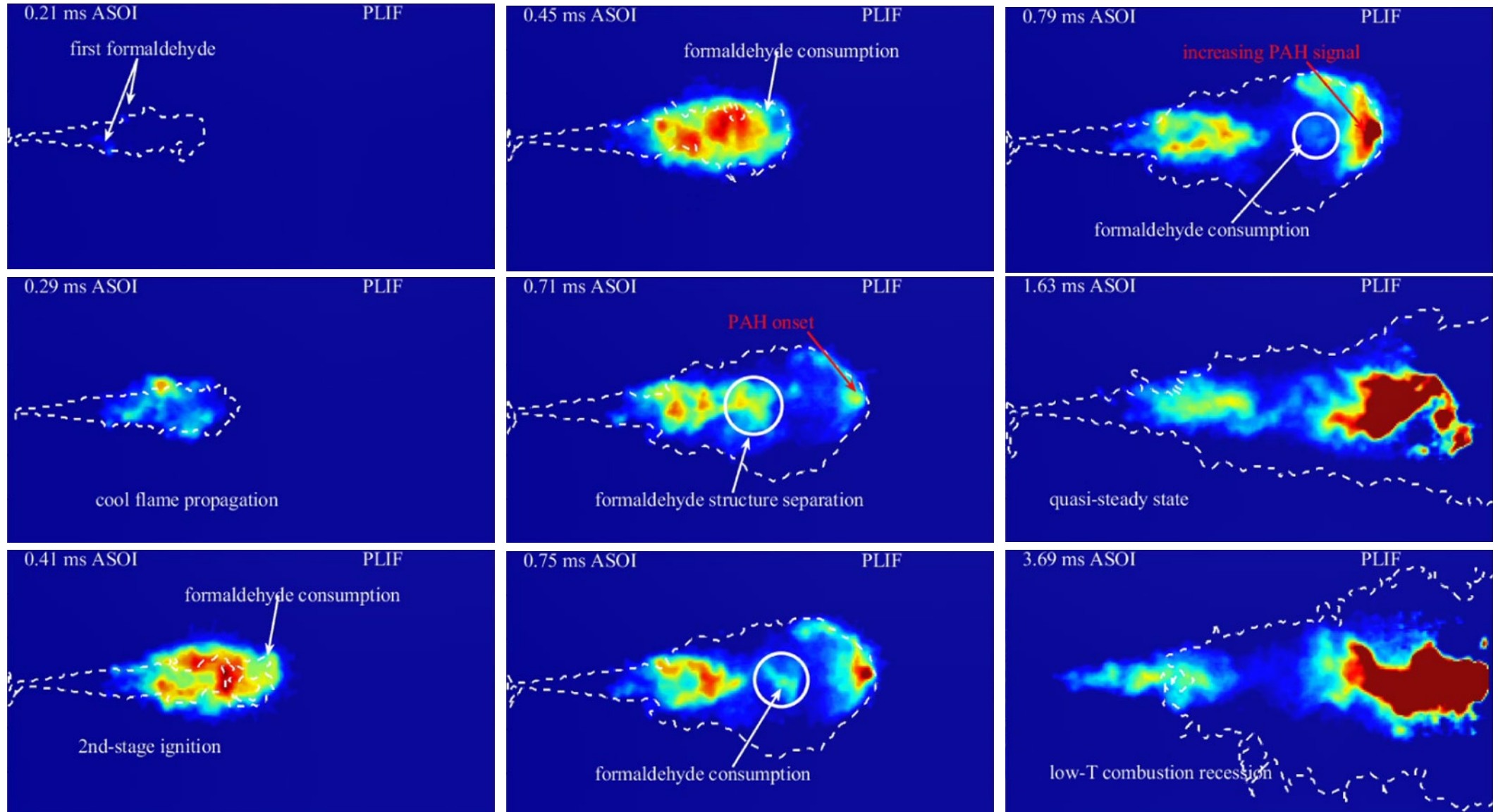
<sup>1</sup>Collaboration with Lukas Weiss at University of Erlangen in Germany

# ① Reference case for 50 kHz planar 355-nm PLIF: Single injection at ECN “Spray A” condition



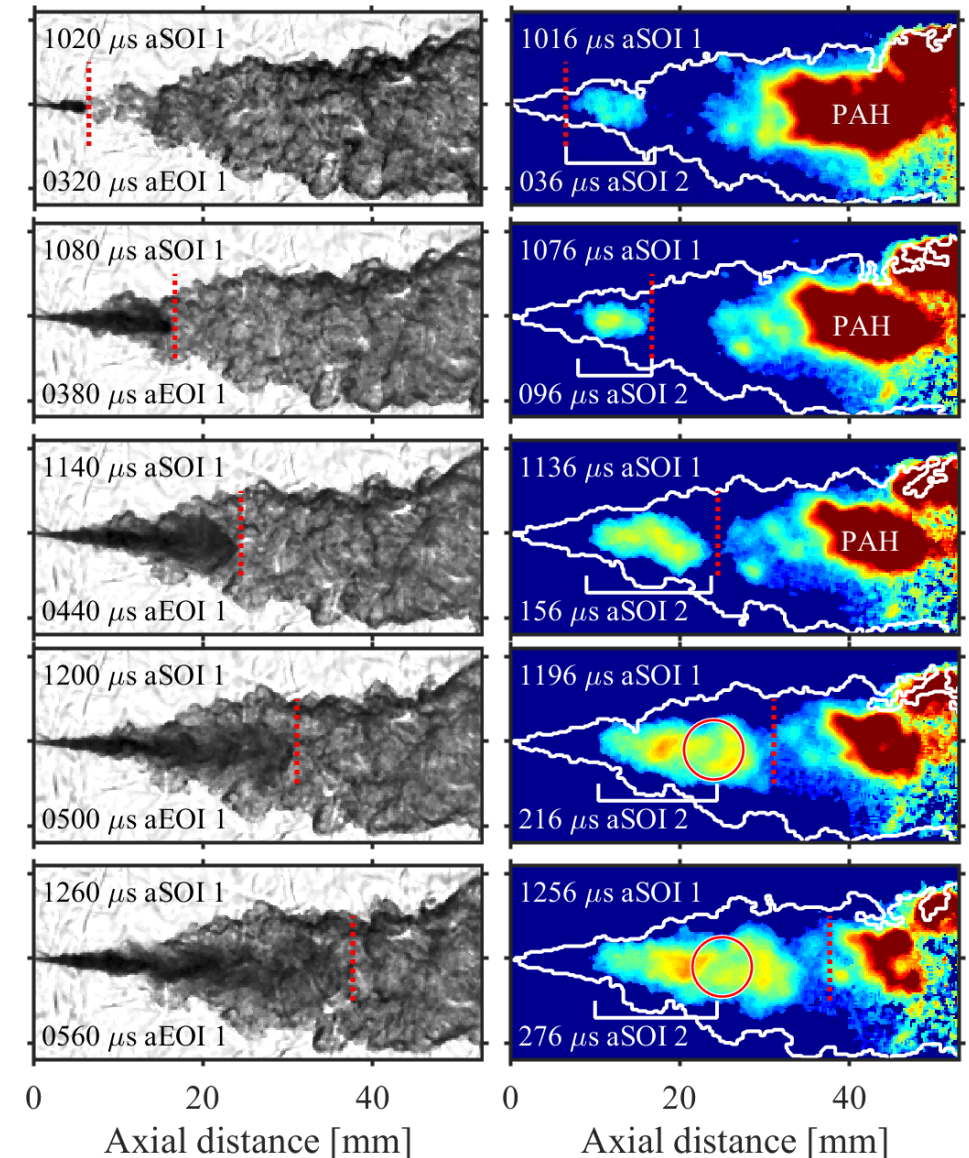


# ① Diesel conceptual model in high-speed 355-nm PLIF: 2-stage ignition, formaldehyde upstream, PAH downstream



# ① Second injection ignites at first-injection's formaldehyde; PAH forms earlier and farther upstream than single inj.

- Multiple-injection schedule:
  - First injection duration: 700 $\mu$ s
  - Dwell between injections: 280 $\mu$ s
  - Second injection duration: 800 $\mu$ s
- Dwell is short enough that 1<sup>st</sup>-stage combustion ( $\text{CH}_2\text{O}$ ) is still receding at start of second injection
- 1<sup>st</sup>-stage  $\text{CH}_2\text{O}$  PLIF signal increases as soon as jet penetrates (red-dotted line) into receding 1<sup>st</sup>-stage combustion products (white brackets,  $\text{CH}_2\text{O}$ )
- In the second injection, the decreasing PLIF signal (circled in red) is consistent with  $\text{CH}_2\text{O}$  consumption and transition to PAH formation downstream
- New  $\text{CH}_2\text{O}$  & PAH PLIF from second injection form closer to orifice than for first injection, then slowly drift downstream toward original quasi-steady location



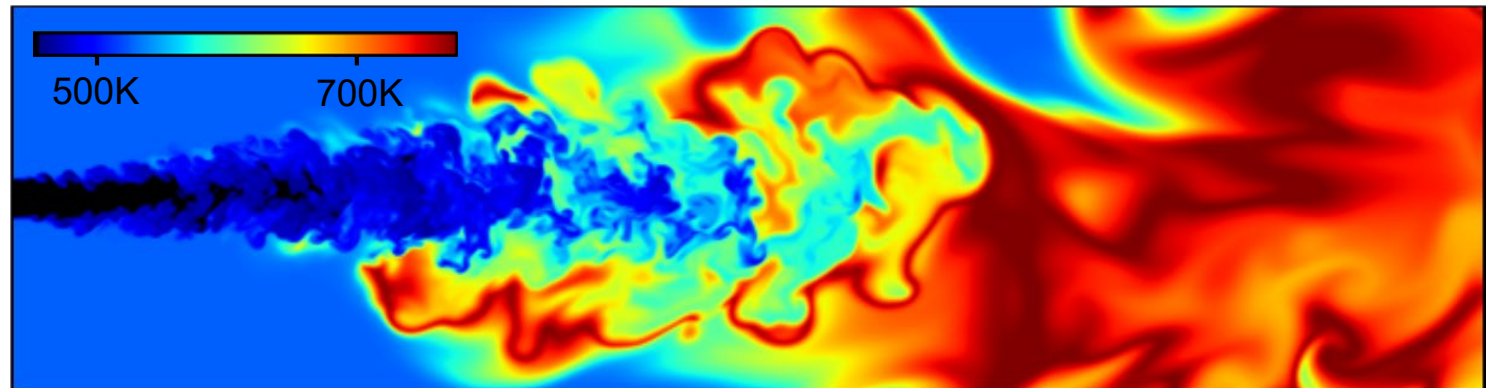
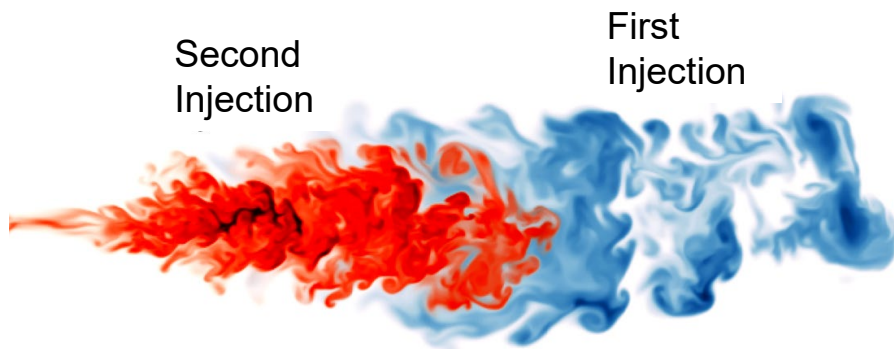


## ② Direct numerical simulation of analogous gas-jet provides additional insight into ignition of second injection

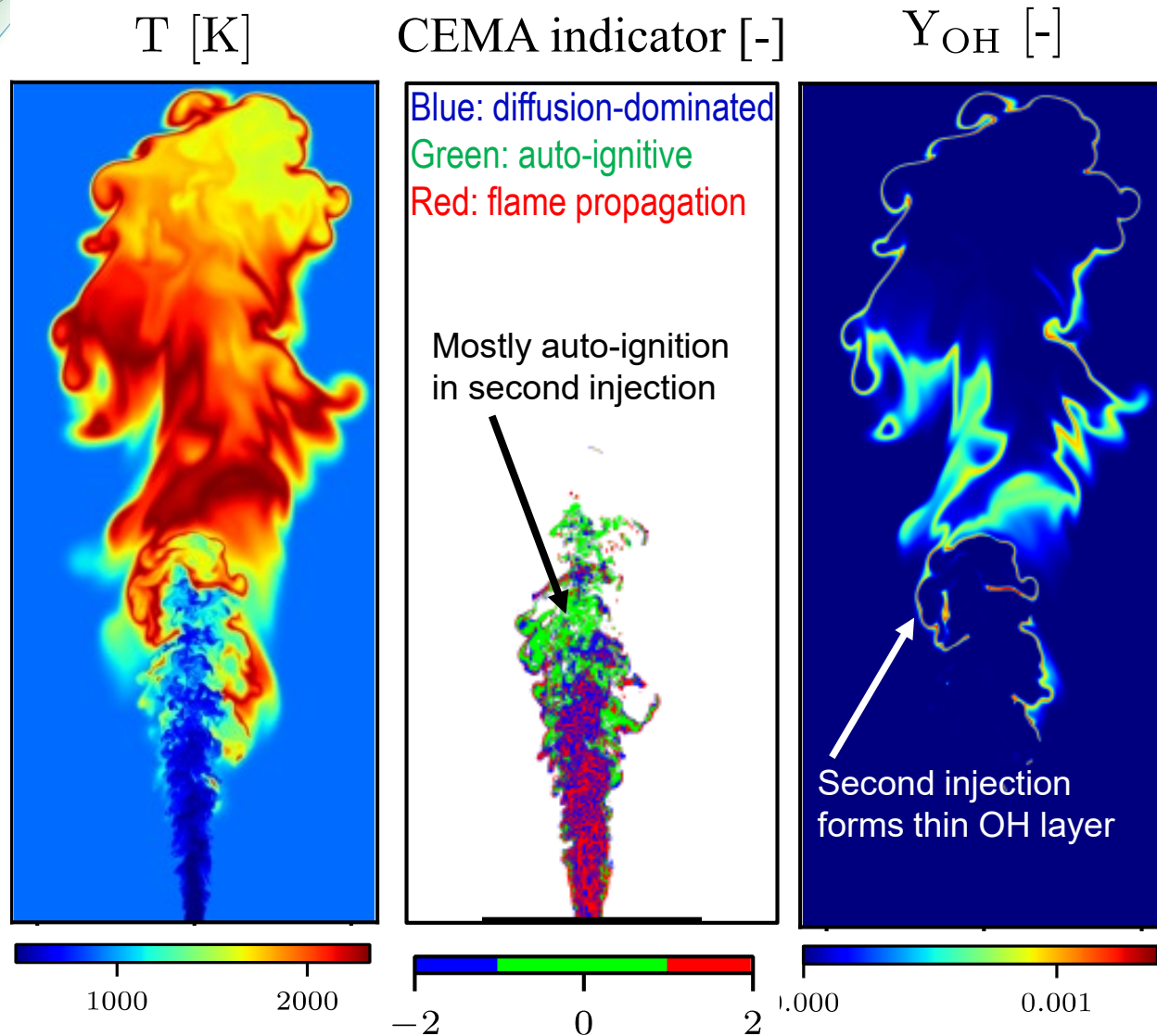
- Analysis of DNS predictions provide insight into mechanism behind experimental observations of 1<sup>st</sup>-stage combustion products of first injection affecting ignition of second injection
  - Is ignition caused by mixing with high temperature products of first-injection combustion, or mixing with radical species, or flame propagation into penetrating second injection?

### DNS setup

- Simplified gaseous pre-vaporized jets, down-scaled compared to experiment (reduced Re)
- PeleLM low-Mach adaptive mesh refinement solver
  - Exascale Computing Project combustion DNS code
- 35 species n-dodecane mechanism with both 1<sup>st</sup> and 2<sup>nd</sup> stage ignition chemistry
  - Borghesi et al., 2018, based on Yao et al., 2017



## ② DNS: Ignition of 2<sup>nd</sup> injection dominated by autoignition, not flame propagation, and by thermal mixing, not radicals



- Second injection (cold, blue) penetrates into and mixes with products from first injection (hot, yellow-red)
- Chemical explosive mode analysis<sup>2</sup> (CEMA) shows ignition is dominated by auto-ignition
  - Separate edge-flame calculations show that ignition of second injection is driven mainly by temperature, not by radical species
- After ignition, second injection forms thin OH layer at head, similar to single injection
- Analysis of cross-scalar dissipation rate shows that upstream ignition is inhibited by strong mixing for the first injection, but strong mixing into 1<sup>st</sup> injection hot products accelerates ignition for 2<sup>nd</sup> injection

<sup>2</sup>Chemical Explosive Mode Analysis (Xu et al., 2019, Lu et al., 2010)

## ② DNS: Flamelet models okay for first injection, but strong tangential diffusion precludes them for second injection

- 1D flamelet models assume differential and tangential diffusion can be neglected

### Generalized flamelet equation

$$\Lambda_{tran}^T = \Lambda_{ND}^T + \Lambda_{TD}^T + \Lambda_{DD}^T + \Lambda_{src}^T$$

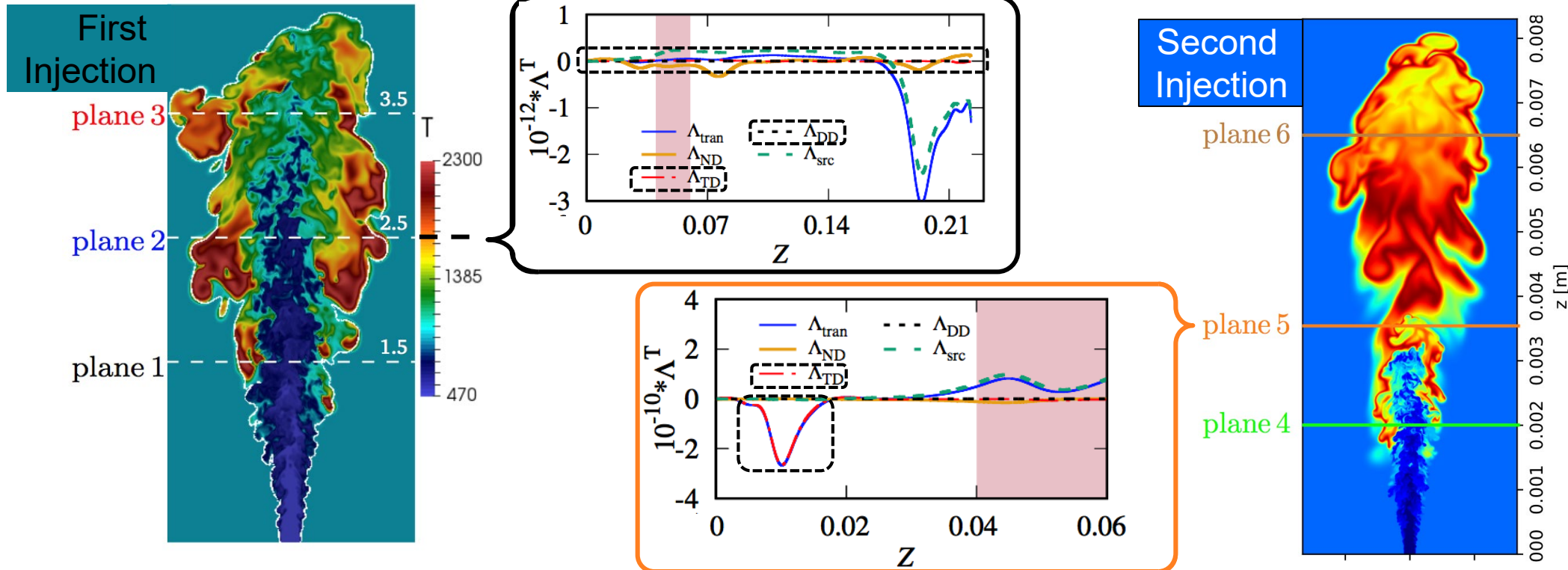
**tran:** transient term, **src:** source term, **ND:** normal diffusion

**TD:** tangential diffusion (typically neglected)

**DD:** differential diffusion (typically neglected)

<sup>3</sup> From collaboration with TU Darmstadt, Wen et al, Proc. Comb. Inst. (2020)

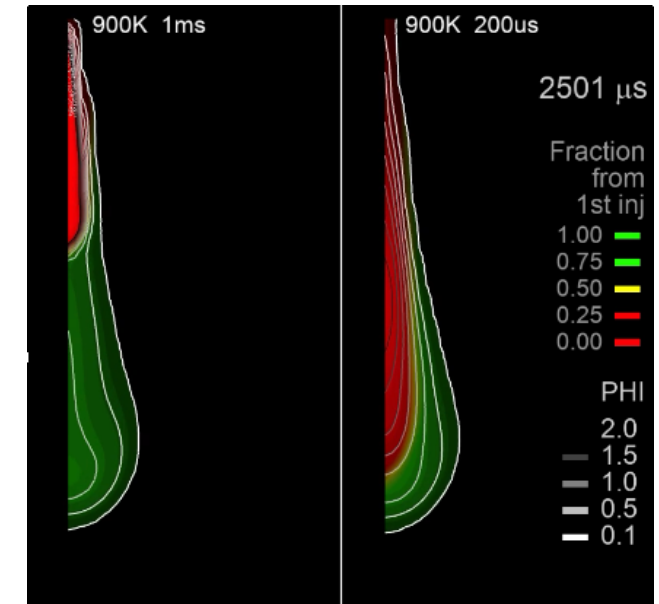
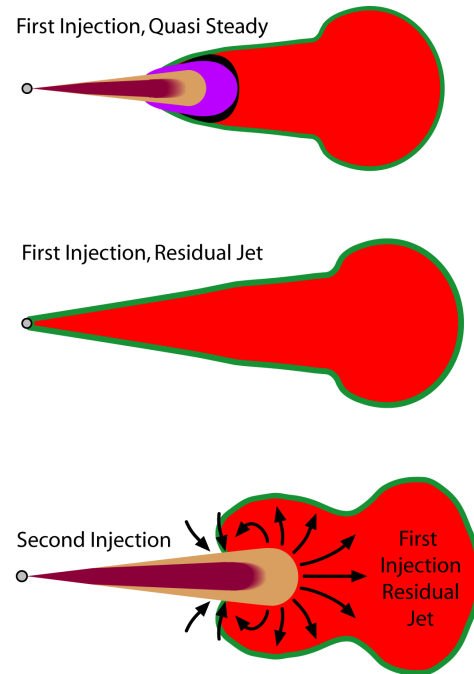
- DNS: 1<sup>st</sup> injection ignition in compressed gas near TDC: 1D assumption is justified<sup>3</sup>
- DNS: 2<sup>nd</sup> injection ignition in 1<sup>st</sup> inj. hot products: tangential diffusion too high for 1D assumption<sup>3</sup>





# ③ RANS: Provide guidance for expts. on multi-inj. effects on fuel distribution & residence times within the combined jet

- Single-injection quasi-steady jet is relatively well understood
- Displacement/mixing of first-injection fuel by second injection is less clear
  - Displacement of 1<sup>st</sup> inj. jet by 2<sup>nd</sup> inj.?
  - How much mixing of 1<sup>st</sup> inj. jet with 2<sup>nd</sup> inj.?
- Use RANS (KIVA) with species tracking tool to distinguish 1<sup>st</sup> injection fuel from 2<sup>nd</sup>
- Complementary to DNS/LES for guiding experiments with ensemble-averaged data
- Four double-injection cases
  - 750 and 900 K, 200 and 1000  $\mu$ s dwell



## Injector conditions

Number of holes / diameter	[ $\mu$ m]	1 / 141
Fuel type		n-dodecane ( $C_{12}H_{26}$ )
Fuel mass injected	[mg]	6.86 total 3.43 per injection
Injection strategies (2)		1.0ms <sub>inj</sub> – 1.0ms <sub>dwell</sub> – 1.0ms <sub>inj</sub> 1.0ms <sub>inj</sub> – 200 $\mu$ s <sub>dwell</sub> – 1.0ms <sub>inj</sub>
Chamber conditions (2)		
CVCC gas temperature.	[K]	900      750
Chamber gas density	[kg/m <sup>3</sup> ]	22      22
Chamber pressure	[bar]	59      49
Chamber gases O <sub>2</sub> /N <sub>2</sub>	[% by vol]	18 / 82      15 / 85

### ③ RANS: Unlike 1<sup>st</sup> inj., 2<sup>nd</sup>-inj. fuel is confined to jet axis; 1<sup>st</sup>-inj. fuel is radially outward & behind 2<sup>nd</sup>-inj. fuel at head

- Non-reacting multiple injection
  - 900K, 1 ms DOI, 0.2 ms dwell, 1 ms DOI
- Radial profiles show fuel mass fraction
  - Green → 1<sup>st</sup> injection
  - Red → 2<sup>nd</sup> injection
- 2<sup>nd</sup> inj. fuel distribution differs from 1<sup>st</sup> inj.
  - As 2<sup>nd</sup> injection (red) advances, its fuel is mostly near the jet axis, while 1<sup>st</sup> injection fuel (green) resides further radially outward
  - 2<sup>nd</sup>-inj. penetrates rapidly to head, expanding radially, leaving 1<sup>st</sup> injection fuel behind
  - Considerable mixing between injections at head and mid-stream axis (red-green overlap)
  - Little mixing in tail near injector (left, red/2<sup>nd</sup>)
  - Little mixing at outer jet behind head (green/1<sup>st</sup>)





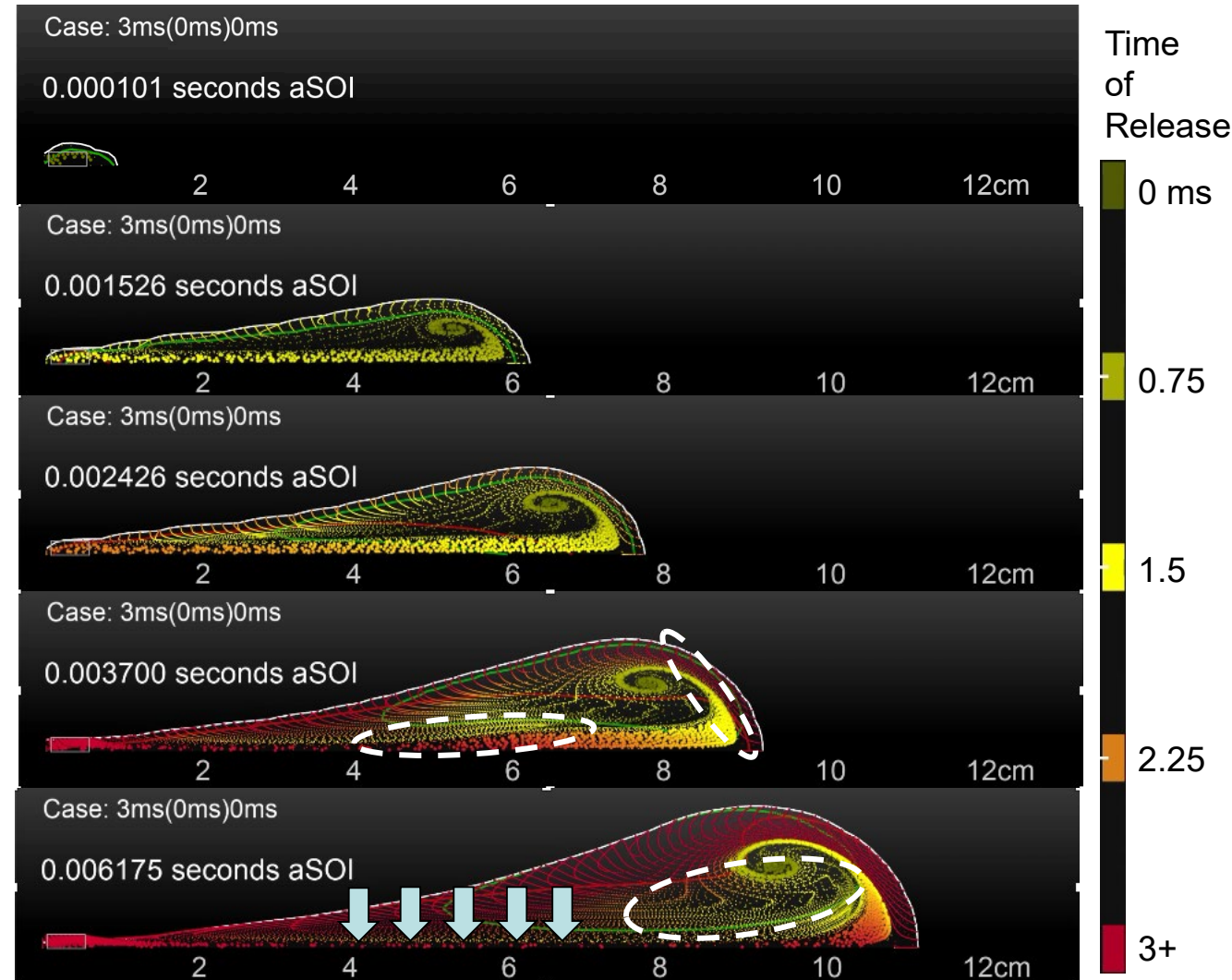
### ③ RANS: Fuel distribution of a single inj. parallels multi-inj.; mean-convection analysis reveals age and flow drivers

- Non-reacting single injection
  - 900K, 3 ms DOI (0 ms dwell, 0 ms DOI2)
- Vapor fuel colored by time in injection:
  - Green → 1<sup>st</sup> half, red → 2<sup>nd</sup> half
- Add flow tracers (“virtual particles”)
  - Carried by mean velocity from nozzle
  - Colored by time of release at nozzle
- Flow tracer age/trajectory insight:
  - Mean velocity confines 2<sup>nd</sup>-half fuel to axis, similar to 2<sup>nd</sup> injection fuel
  - Turb. mixing helps distribute fuel radially
  - Older tracers accumulate in head vortex
  - Newer tracers rapidly advance to jet tip
  - After EOI, tracers narrow along jet axis
    - Increased radial entrainment?



### ③ Mean velocity entrains gas near axis; head has oldest entrained gas, new entrained gas near older injected fluid

- Non-reacting single injection
  - 900K, 3 ms DOI (0 ms dwell, 0 ms DOI2)
- Two types of flow tracers
  - Large: Released near nozzle
  - Small: Released at jet boundary
- Flow tracer entrainment insight:
  - Mean velocity carries ambient gas (small tracers) deep into jet (large tracer bound.)
    - Pushes injected fluid toward axis after EOI
  - Older entrained gas also at jet head
  - Newer entrained gas in proximity with older injected fluid along axis & at jet tip
    - Residence time implications for chemistry
  - Entrainment along whole jet boundary, even at jet tip (ensemble-avg. aspect)





## ④ RANS analysis: need experiments to track 1<sup>st</sup>- and 2<sup>nd</sup>-inj. fuel separately; one option: laser-induced phosphorescence

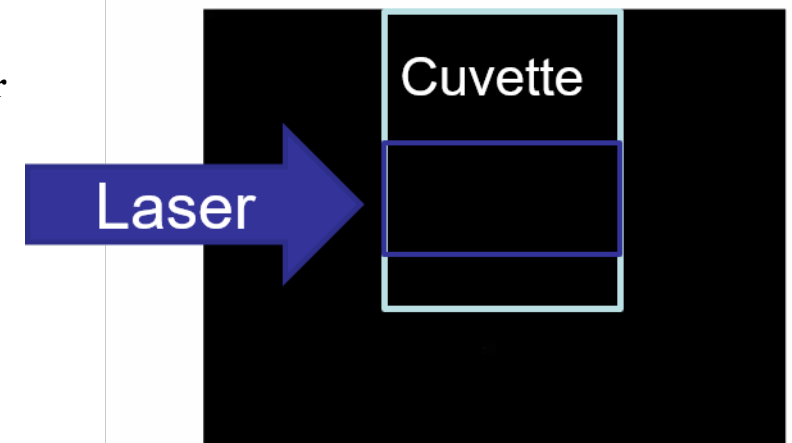
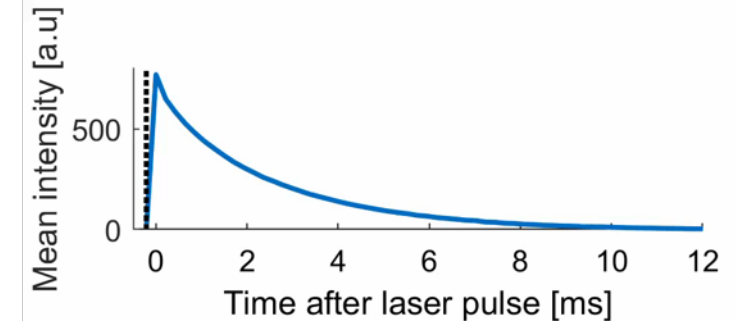
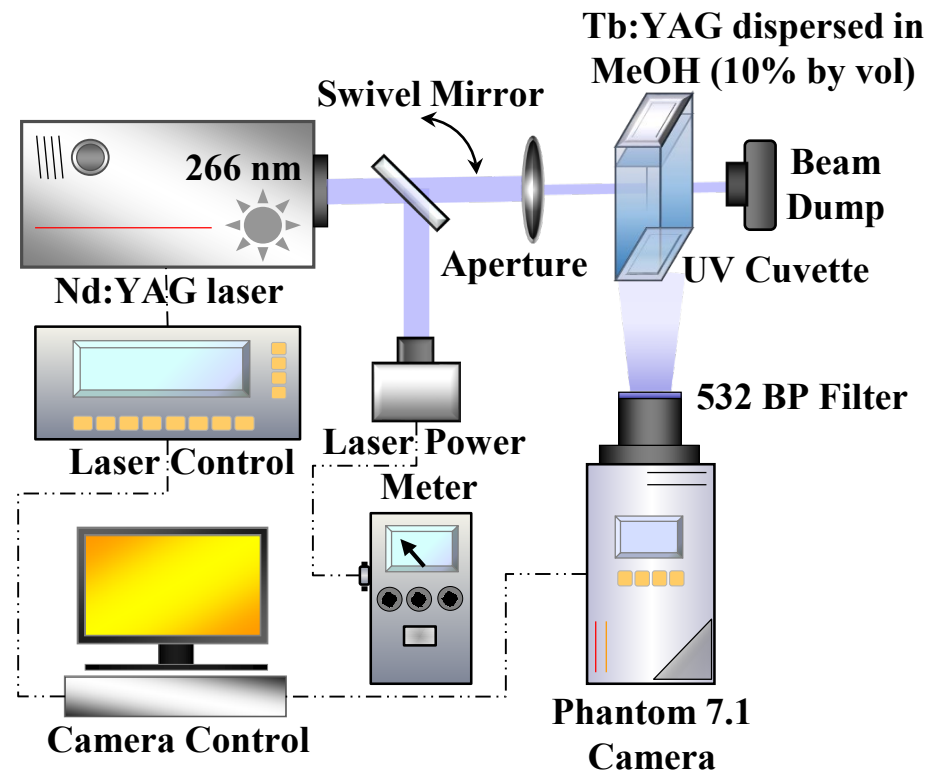
- RANS predicts areas of both mixing and stratification of fuel from multi-injections
  - Guides experiments on need to measure fuel from first and second injection separately
- One laser-imaging diagnostic: Planar Laser-Induced Phosphorescence (PLIP)
  - For reference, laser-induced fluorescence of gas-phase species (OH, CH<sub>2</sub>O, PAH, toluene, acetone, etc.) has typical signal lifetimes of 10-1000 ns at compressed in-cylinder conditions
  - Laser-induced phosphorescence of solid particles can have lifetimes of 0.1-10 ms
  - Long-lived phosphorescence can show later location of “tagged” first-injection fuel
- Gas-phase example: Eu-doped particles aerosolized for PIV<sup>4</sup> (0.9 ms lifetime at room T)<sup>5</sup>
  - Simultaneous temperature and velocity imaging using a single laser, and color camera
- Liquid-phase example: Eu-doped particles suspended in polar and non-polar solvents<sup>6</sup>
  - Particles laser-tagged in a 100 bar water jet show velocity, change in structure, and qualitative indication of dispersion as the jet breaks up
  - Heptane and water-ethanol laser-tagged inside a 200 μm nozzle show the displacement and structure of the tagged fluid 183 μs after laser excitation

<sup>4</sup>Yokomori et al, SAE Tech. Paper 2015-01-2002 (2015)   <sup>5</sup>Choy et al, J. Mat. Res. 14(7):3111-3114 (1999)   <sup>6</sup>Van der Voort DD et al., Atomiz. Sprays 26(3):219-233 (2016)

# ④ Tb-doped YAG particles selected as best candidate for sufficient lifetime at high in-cylinder temperatures near TDC

- Literature survey of phosphor candidates: terbium-doped yttrium-aluminum-garnet (Tb:YAG) has longest known lifetime at high T (~900K)
  - Tb:YAG nanoparticles can be suspended in polar solvents for fuel tracer experiments
- Bench-scale feasibility experiments using fused-silica cuvette<sup>7</sup>
  - Suspensions in non-polar solvents are not sufficiently stable
  - Tb:YAG in methanol has good lifetime and stable suspension
  - Go/no-go: proceed to engine tests**

Phosphor	Tb:YAG
Particle size	35-40 nm (est.)
Excitation $\lambda$	266 nm (UV)
Emission $\lambda$	Peak at 544 nm
Emission lifetime	~2 ms at 300K
Phosphor mixture	10% (vol.) in Methanol



<sup>7</sup>Collaboration with Ted Lind at Lund University in Sweden

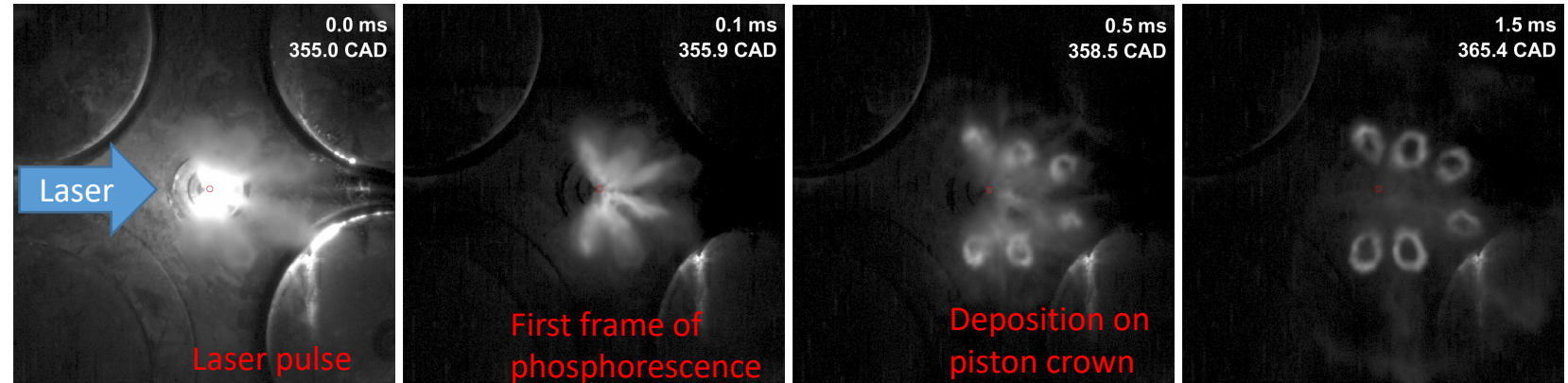


## ④ PLIP in engine with narrow-angle GDI shows sufficient lifetime for 1<sup>st</sup> injection tracing; challenges remain

- PLIP of Tb:YAG by narrow-angle GDI: sufficient lifetime (1ms+) for tracking multiple injections
  - Particles deposited on relatively cool piston window for TDC injection have longer lifetime
- Many challenges remain, including maintaining suspension, avoiding diesel injector clogging, improving S/N, extending to non-polar solvents, characterizing/quantifying decaying signal, etc.

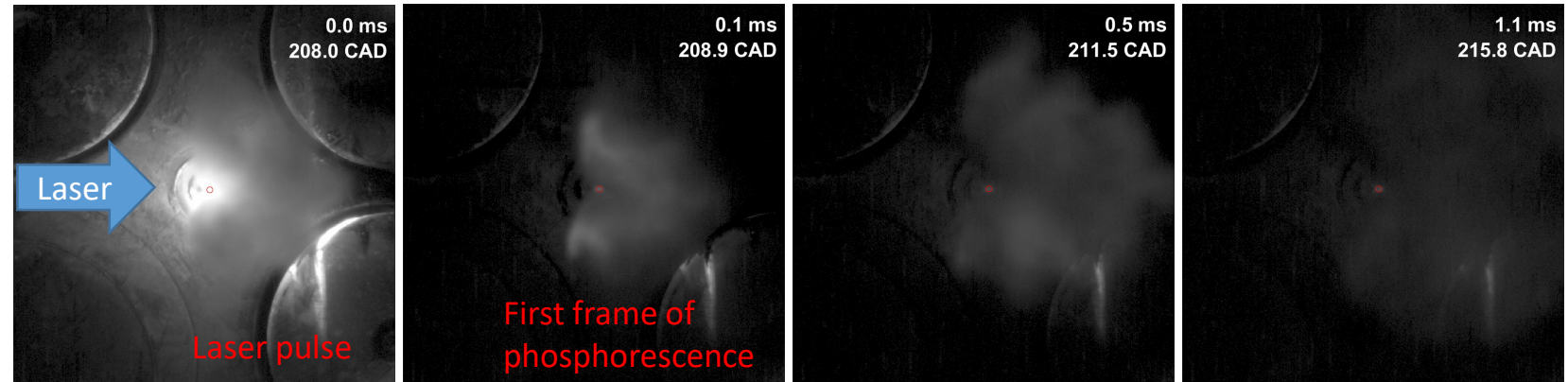
Near-TDC  
100-bar GDI,  
MeOH into  
900K air

Tb:YAG/Methanol  
SSE=200CAD  
DSE=2ms  
Laser@355CAD  
 $T_{in}=100C$   
 $P_{in}=1bar$   
Gamma=2.5  
-0.5 ms  
351.5 CAD



Start of  
compression  
100-bar GDI,  
MeOH into  
400K air

Tb:YAG/Methanol  
SSE=200CAD  
DSE=2ms  
Laser@208CAD  
 $T_{in}=100C$   
 $P_{in}=1bar$   
Gamma=2.5  
-0.5 ms  
204.5 CAD







# Remaining Barriers/Future Plans: Continue to develop conceptual models for HT and multiple injections

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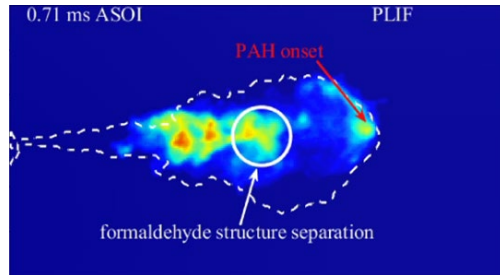
Back-and-forth exchanges between simulations and experiments help to guide new measurements to develop design guidance and conceptual model across multiple modes and multiple injections for CDC and LTC

- Laser/imaging experiments in engines and chambers to continue to contrast physical and fuel inter-mixing effects of multiple injections with those of single injections, including swirl, spray-generated turbulence, entrainment-wave, and roles of large-scale structures
- Further laser/imaging experiments to understand how mixing processes specific to multiple injections affect the thermal and chemical coupling between injections affecting ignition, combustion, and emissions, including simultaneous high-speed PAH PLIF and soot DBI with primary reference fuels where only one of the fuels has low-temperature chemistry
- Use DNS multi-injection diesel data to train and evaluate supervised (labeled data from CEMA or PCA analysis) and unsupervised machine learning to develop models for LES/RANS
- Use DNS multi-injection data develop multi-injection flamelet model using 'age' variable as a residence time marker with a single mixture fraction instead of  $n$  mixture fractions  $n$  injections
- Continue constructing RANS simulation cases to complement experimental measurements and re-apply recently developed analysis tools to contribute to a multiple injection conceptual model

*\* Any proposed future work is subject to change based on funding levels*

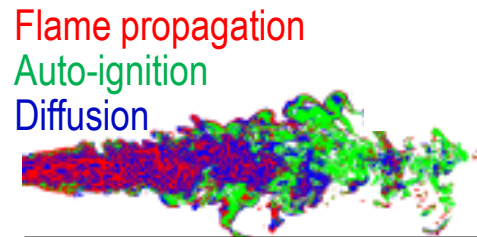
# Summary - ACE001 - Heavy-Duty Diesel Combustion

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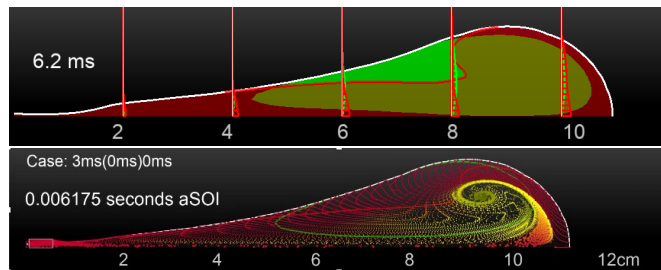
50 kHz planar 355-nm PLIF reveals key diesel conceptual model features within a single injection event, but with new cause-effect evidence of structure evolution. For multiple injections, the second injection strengthens receding 1<sup>st</sup>-stage ignition from first injection, leading to transient upstream shift in ignition and PAH formation.

②



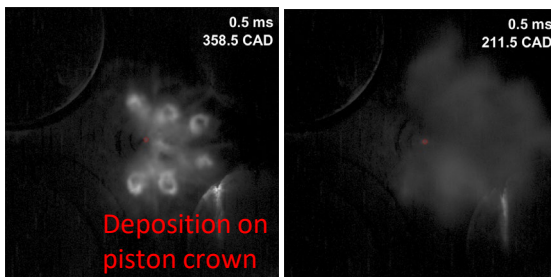
Chemical explosive mode analysis of multiple-injections in DNS shows ignition of second injection is dominated by auto-ignition, driven mainly by temperature, not radicals. 1D flamelet-model assumptions are justified for the first injection, but not for the second injection

③



Non-reacting RANS simulations to guide experiments predict 2<sup>nd</sup>-injection fuel mostly near jet axis, while 1<sup>st</sup>-injection fuel resides further radially outward. Little mixing in tail or behind head vortex, but new entrained gas is brought in close proximity to older injected fuel along jet axis and near jet tip.

④



Planar laser-induced phosphorescence (PLIP) of narrow-angle GDI using Tb:YAG nanoparticles suspended in MeOH demonstrated sufficient lifetime (1ms+) for tracking fuel separately from multiple injections. Challenges remain for quantitative measurements, but could enable new understanding of multi-injection mixing.